Comment on "Feshbach-Einstein condensates" by V. G. Rousseau and P. J. H. Denteneer

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In a recent letter [1], making use of quantum Monte Carlo (QMC) simulations Rousseau and Denteneer (RD) have investigated a two-species Bose-Hubbard (BH) model in a one-dimensional optical lattice, with coherent conversion between two particles of a species and one of the other, mimicking the atom-molecule coherence occurring in cold gases in optical lattices close to a Feshbach resonance [2, 3]. In the notation of Ref. 1, the Hamiltonian under investigation is

$$\mathcal{H} = -t_a \sum_i \left(a_i^\dagger a_{i+1} + \text{h.c.} \right) - t_m \sum_i \left(m_i^\dagger m_{i+1} + \text{h.c.} \right)$$
$$+ U_{aa} \sum_i n_i^{(a)} \left(n_i^{(a)} - 1 \right) + U_{mm} \sum_i n_i^{(m)} \left(n_i^{(m)} - 1 \right)$$
$$+ U_{am} \sum_i n_i^{(a)} n_i^{(m)} + D \sum_i n_i^{(m)} + g \sum_i \left(m_i^\dagger a_i^2 + \text{h.c.} \right) \quad (1)$$

where t_a and t_m are the atomic and molecular hoppings, U_{aa} and U_{mm} are the interatomic and intermolecular interactions, U_{am} is the atom-molecule interaction, D is the "detuning" between atomic and molecular states (the true detuning being $D - U_{aa}$) and g is the amplitude of atom-molecule conversion. This model was previously investigated by the same authors in Ref. 4 for a large variety of parameters.

One of the main claims of Ref. 1 is the existence of a novel phase, dubbed *super Mott* (SM), which is characterized by zero compressibility (namely absence of fluctuations in the total particle number $N = N_a + 2N_m$) and finite superfluid fraction of both the atoms (ρ_s^a) and the molecules (ρ_s^m). Moreover, the superflows of atoms and molecules appear to be anticorrelated, namely the correlated superfluid density (ρ_s^{cor}) turns out to be zero. In this comment we argue that the claimed SM phase does *not* contain any superfluid component, and that the individual superfluid densities of atoms and molecules ρ_s^a and ρ_s^m are not well defined in the model of Eq. (1). In fact, the only meaningful superfluid density is the correlated one ρ_s^{cor}, which turns out to be vanishing, revealing a normal phase. We corroborate the above statement with the explicit numerical calculation of the correlation function associated with the coherent counterflow of atoms and molecules, and we show that this correlator is short-ranged in the supposed SM region.

At $T = 0$ the superfluid density of one bosonic species is defined via the energy cost of a boost in the phase of the operators associated to that species. E.g. for the atoms, considering the phase shift $a_j \rightarrow a_j e^{i\phi j}$, one defines $\rho_s^a = \frac{1}{2L} \partial^2 E_0 / \partial \phi^2 |_{\phi=0}$ (where E_0 is the ground state energy and L is the size of the system). For a single species BH model, the explicit calculation of the superfluid density within the path-integral formalism shows that this quantity can be estimated via QMC simulations on a system with periodic boundary
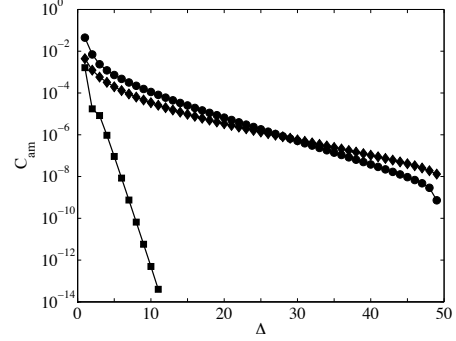

FIG. 1: Atom-molecule correlator for a $L = 100$ chain with parameters: $(D/t_a, \mu/t_a) = (3, 8.6)$ [squares], $(7, 9.6)$ [circles], $(13, 10.6)$ [diamonds]. The other parameters are $U_a = 8t_a$, $U_{am} = 12t_a$, $U_m = \infty$, $g = 0.5t_a$, $t_m = 0.5t_a$. According to Fig. 10 of Ref. 4 all three parameter sets should give a SM phase .

conditions by means of the fluctuations of the winding number (W) of the worldlines associated with the motion of particles in imaginary time [5, 6]. When particle-number conservation holds — as in the single-species BH model — supercurrents are topological invariants (independent of the connected surface through which the current is measured), and indeed so is the winding number for each configuration sampled by the Monte Carlo. Yet in the case of Eq. (1), the atom and molecule numbers are not conserved separately, so that neither the currents of each species are not topological invariants nor the atomic and molecular winding numbers, W_a and W_m. The only conserved quantity is the total number N, and hence the only meaningful superfluid density is the one associated with the correlated superflow of atoms and molecules, captured by the correlated winding number $W_{\text{cor}} = W_a + 2W_m$ introduced in Refs. 1, 4. From a technical point of view, this corresponds to the fact that an arbitrary phase boost of the operators, $a_j \rightarrow a_j e^{i\phi_a j}$, $m_j \rightarrow m_j e^{i\phi_m j}$, produces a rotation of the atom-molecule conversion term $m_j^\dagger a_j^2 \rightarrow m_j^\dagger a_j^2 e^{i(2\phi_a - \phi_m)j}$ which grows with the position j (hence leading to an energy variation in the ground state which is not infinitesimal in the limit $\phi_{a,m} \rightarrow 0$), unless $\phi_m = 2\phi_a$, which corresponds to probing the correlated response of atoms and molecules, namely the correlated superfluid density. In fact, following Refs. 5, 6 it is straightforward to prove that the correlated superfluid density, defined in Ref. 1 as $\rho_s^{\text{cor}} = \lim_{T \rightarrow 0}(k_B T L/2)\langle W_{\text{cor}}^2 \rangle$, can be written as $\rho_s^{\text{cor}} = \frac{1}{2L} \partial^2 E_0 / \partial \phi_a^2 |_{\phi_a=0}$ with the correlated boost $\phi_m = 2\phi_a$. Hence the only meaningful superfluid density is the correlated one; which, as shown in Refs. 1, 4, is perfectly vanishing in the SM phase. Consequently the supposed SM phase is actually *normal*, and its name is misleading.

As argued in Refs. 1, 4, the superfluid nature of the SM phase stems from counterflow of pairs of atoms and molecules, leading to a zero net mass current. Counterflow superfluidity (CSF) has been theoretically predicted in repulsive binary mixtures of bosons (with particle number conservation of both species) and it is associated to condensation (or quasi-condensation in one dimension) of composite objects made of one particle of a given species and one hole of the other species [7, 8]. In analogy to CSF, if the SM phase contained counterflowing superfluid components, one would then expect composite objects made of two atoms and a molecular hole — or of two atomic holes and one molecule — to quasi-condense. We have explicitly checked this by investigating the atom-molecule correlation function $C_{am}(\Delta) = \langle (a^\dagger_{L/2})^2 m_{L/2} m^\dagger_{L/2+\Delta} (a_{L/2+\Delta})^2 \rangle - \langle (a^\dagger_{L/2})^2 m_{L/2} \rangle \langle m^\dagger_{L/2+\Delta} (a_{L/2+\Delta})^2 \rangle$ for parameters which are claimed by RD to correspond to a SM phase. Fig. 1 shows the above quantity calculated numerically by a variational Matrix Product State Ansatz [9] with bond dimension $D = 60$, for a chain of length $L = 100$ with open boundary conditions; all the parameters are chosen so as to be in the SM phase (according to Fig. 10 of Ref. 4) and close to the resonance condition $D = U_a$. We find that the C_{am} correlator decays *exponentially* for all the investigated parameters, as well as all the correlators to lower order. Hence no quasi-condensation phenomenon is observed in the supposed SM phase, confirming its fully normal character.

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